

Quantum Spin Chains and Ladders: Theoretical Concepts and Recent Developments

H.-J. Mikeska

Institut für Theoretische Physik

Universität Hannover 

Outline

- 1 Introduction
- 2 prototypes of low D magnets
- 3 low D quantum magnets in an external magnetic field
- 4 multi spin interactions
- 5 excitation continua
- 6 Summary

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Milestones in Low D Magnetism

- 1925/31 Ernst Ising, Hans Bethe (Heisenberg chain)
- 1944 Lars Onsager: 2D Isingmodell
- 1966 Mermin-Wagner theorem: **strong temperature fluctuations**
- 1971 Baxter: Eight vertex model

Milestones in Low D Magnetism

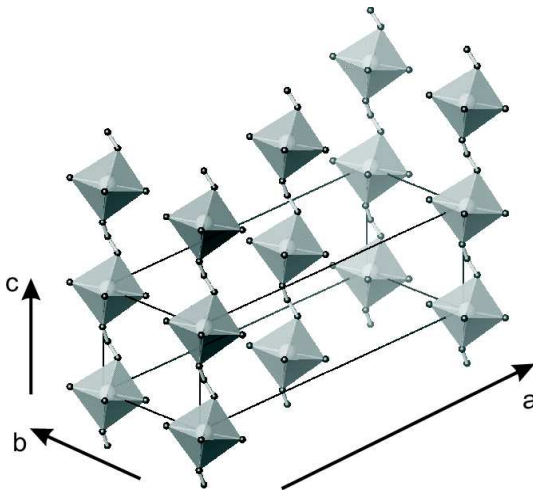
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- 1983 Haldane conjecture: strong quantum fluctuations
- 1986 High T_c superconductivity based on 2D AF's

Milestones in Low D Magnetism

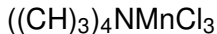
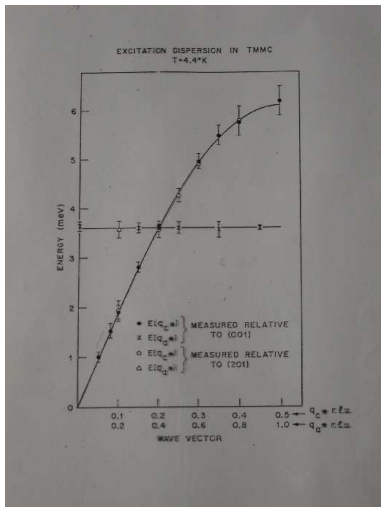
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- 1986 High T_c superconductivity based on 2D AF's
- since 1990 quantum phase diagrams / magnetization plateaus
order from disorder / BEC of quantum magnets /
quantum solitons

Low-dimensional magnets exist as real crystals

example: $\text{Ni}(\text{C}_5\text{H}_{14}\text{N}_2)_2\text{N}_3(\text{ClO}_4) = \text{NDMAZ}$



experimental check of low dimensionality



= TMMC

$$S = \frac{5}{2}$$

inelastic neutron
scattering:

Hutchings, Shirane,
Birgeneau and Holt
(1972)

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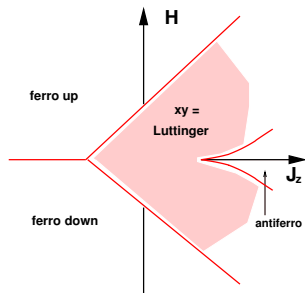
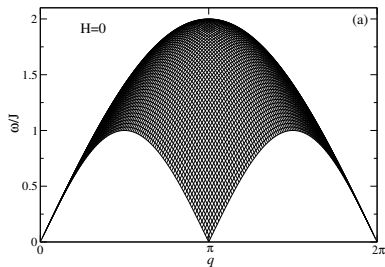
prototypes of low dimensional magnets:

- **S=1/2 Heisenberg chain**
- 1D quantum spin systems with gap and rotationally invariant exchange
- $S = 1/2$ chain with orbital degree of freedom
- 2D S=1/2 Heisenberg magnets

low D prototypes (1): $S=1/2$ Heisenberg chain

$$\mathcal{H} = \sum_n J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + J_z S_n^z S_{n+1}^z - H \sum_n S_n^z$$

$-J < J_z < +J$: gapless algebraic spin liquid / **excitation continuum**
 interacting fermions
 with **non Fermi (Luttinger) liquid** behaviour



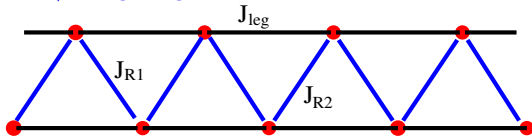
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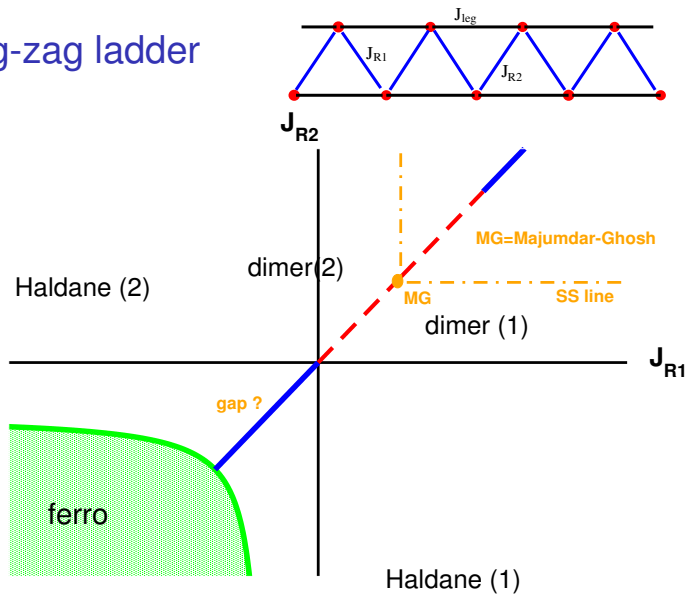
low D prototypes (2): 1D quantum spin systems with gap and rotationally invariant exchange

- $S = 1$ Heisenberg antiferromagnet: Haldane gap $\Delta \approx 0.41..J$
- $S = 1/2$ HAF with NN exchange J and NNN exchange J_2 :
 $J_2 > 0.2411...J$: excitation gap, 2 degenerate ground states
 $J_2 = 0.5J$: Majumdar-Ghosh chain (exact dimer ground states)
 $0.5J < J_2 < 1.25J$: **magnetization plateau** at 1/3 saturation
- $S = 1/2$ two leg ladder: excitation gap $\Delta \approx 0.5J$

unified view: $S = 1/2$ zig-zag ladder



zig-zag ladder



prototypes of low dimensional magnets:

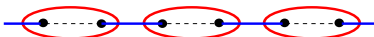
- $S=1/2$ Heisenberg chain
- 1D quantum spin systems with gap and rotationally invariant exchange: **dimer aspects**
- $S = 1/2$ chain with orbital degree of freedom
- 2D $S=1/2$ Heisenberg magnets

dimer aspects of gapped spin systems

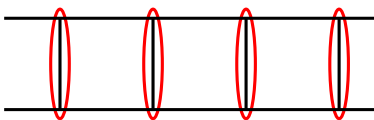
$$S = \frac{1}{2} \text{ dimer: } \mathcal{H} = J \mathbf{S}_1 \cdot \mathbf{S}_2 \quad \implies \Delta E = J$$

$$\text{interacting } S = \frac{1}{2} \text{ dimers: } \mathcal{H} = J \sum_{\vec{n}} \mathbf{S}_{\vec{n},1} \cdot \mathbf{S}_{\vec{n},2} + J' \dots$$

dimer aspect of
 $S = 1$ (Haldane) chain:
 valence bond picture:



dimer aspect of
 two leg ladder:



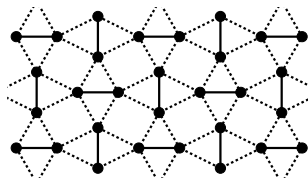
lowest excited state is triplet \approx excited dimer

dimers interacting in 2D / 3D

orthogonal dimers in 2D

($\text{SrCu}_2(\text{BO}_3)_2$):

exact dimer ground state
magnetization plateaus



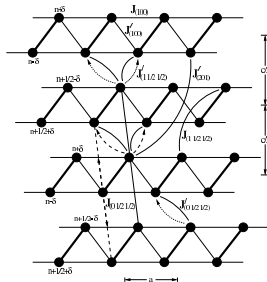
interacting dimer type ladders

(KCuCl_3 , TlCuCl_3 , NH_4CuCl_3):

magnetization plateaus

triplet condensation:

'BEC of magnons'



zigzag ladder in a magnetic field

NN and NNN
exchange:

$$\mathcal{H} = \sum_n (J \vec{S}_n \cdot \vec{S}_{n+1} + J_2 \vec{S}_n \cdot \vec{S}_{n+2} - \mu H S_n^z)$$

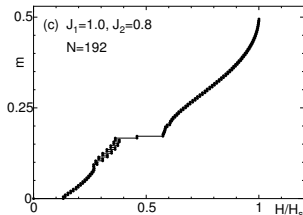
magnetization plateau exists:

$\rho(S - m)$ is integer:

$\rho = 3, S = 1/2, m = 1/6$

Okunishi and Tonegawa, PRB '03;

Yamanaka, Oshikawa, Affleck, PRL '97



zigzag ladder in a magnetic field

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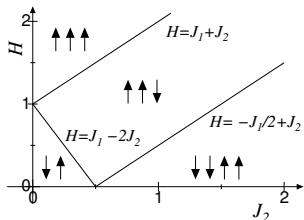
magnetization plateau exists:

$p(S - m)$ is integer:

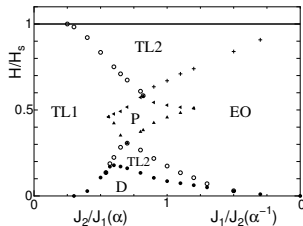
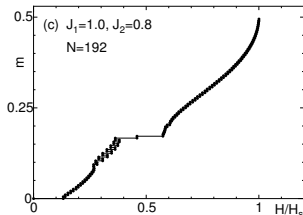
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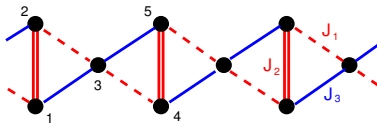
Ising



Heisenberg

$\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2 = \text{azurite}$: a real material

distorted diamond chain:

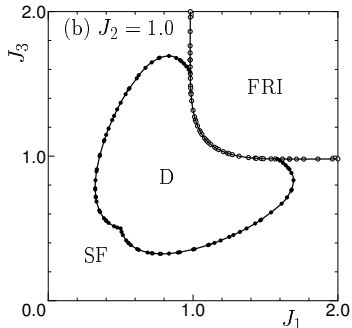


alternative view:

chain with NN interactions
and NNN interactions

$$(J_1 \ J_2 \ J_1)$$

$$(J_3 \ 0 \ J_3)$$



prototypes of low dimensional magnets:

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- 2D $S=1/2$ Heisenberg magnets

low D prototypes (3): $S = 1/2$ chain with orbital degree of freedom

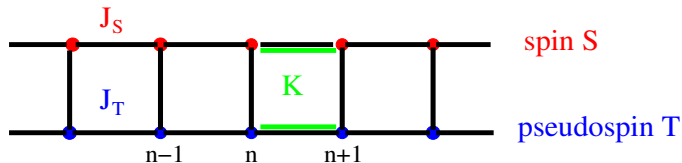
$$\mathcal{H} = J_S \sum_n (\mathbf{S}_n \cdot \mathbf{S}_{n+1}) + J_T \sum_n (\mathbf{T}_n \cdot \mathbf{T}_{n+1}) + K \sum_n (\mathbf{S}_n \cdot \mathbf{S}_{n+1})(\mathbf{T}_n \cdot \mathbf{T}_{n+1})$$

Kugel-Khomskii model:

electron with two orbital states at each site, $S=1/2$, $T=1/2$

\equiv spin ladder with leg-leg biquadratic interaction

$$\left\{ U(\text{same orbital}), U'(\text{different orbitals}), J(\text{Hund}) \right\} \cong \left\{ J_S, J_T, K \right\}$$

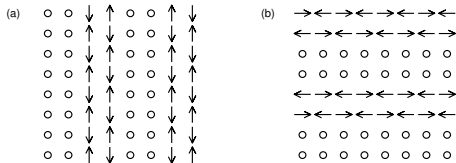


prototypes of low dimensional magnets:

- $S=1/2$ Heisenberg chain
- 1D quantum spin systems with gap and rotationally invariant exchange
- $S = 1/2$ chain with orbital degree of freedom
- **2D $S=1/2$ Heisenberg magnets**

low D prototypes (4): 2D $S = 1/2$ Heisenberg antiferromagnets

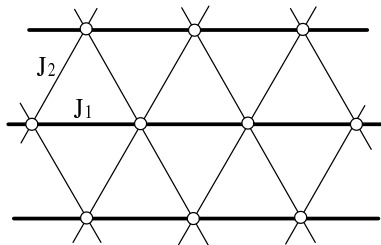
- square lattice with NN exchange (La_2CuO_4):
 - Néel phase with long range order and spin waves
 - four spin (ring) exchange at higher energies
- doped square lattice ($\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, HTSC):
 - charges induce stripes / ladder character



J.S. Tranquada, '05

2D lattices with frustration:

- square lattice with NN and NNN exchange: ▶ ...
satisfies **purist's view of a spin liquid phase: no dimer aspects**
- triangular lattice with spatial anisotropy (Cs_2CuCl_4):
spin liquid / 2D spinons (?)



Coldea, Tennant, Tylczynski '00, '03 ...

quantum phases in localized spin systems

quantum phases differ in

groundstates: ferro-, antiferro, chiral order

disorder: dimers, spin liquid

Heisenberg, XY, Ising symmetry

excitations **spinons** (the quarks of Solid State Physics)

excitation gaps for isotropic interactions

quantum solitons

tune through quantum phase diagrams by varying

materials, doping, pressure **and magnetic field**

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realize external magnetic fields

high magnetic field: $\mu H \approx \mathcal{O}(J) \approx \mathcal{O}(\text{meV})$

for $g = 2.2$: $1 \text{ meV} \approx 8 \text{ T}$, $1 \text{ K} \approx 0.7 \text{ T}$

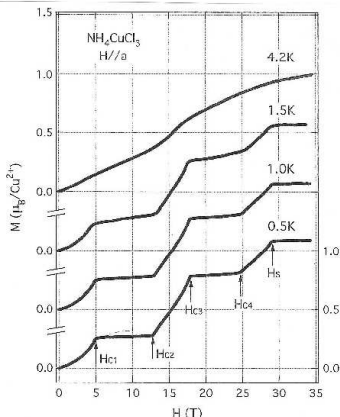
specific heat, magnetization:
up to 90 T (Tokyo)

NMR, ESR:
up to 35 T (Grenoble)

x-ray-, neutron scattering:
up to 15 T (Berlin)

example:
magnetization plateaus
in NH_4CuCl_3

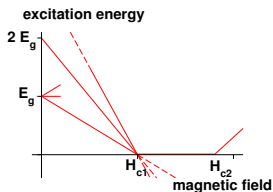
Shiramura, Tanaka '97



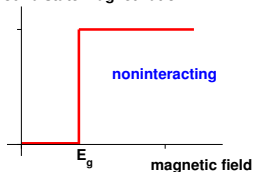
dimer condensation in magnetic field

$$\mathcal{H} = J \sum_{\vec{n}} \mathbf{s}_{\vec{n},1} \cdot \mathbf{s}_{\vec{n},2} + \sum_{\vec{n}, \vec{n}'} J' \dots - H \sum_{\vec{n}, \alpha} S_{\vec{n}, \alpha}^Z$$

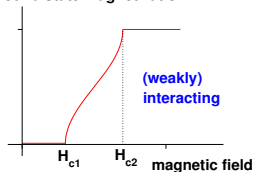
triplet excitation gap
closes at $H = H_{c1} = E_g$
saturation at H_{c2}



ground state magnetization



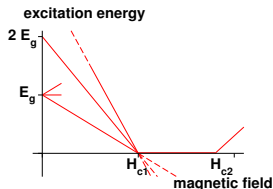
ground state magnetization



Magnetic field: Haldane meets Luttinger

when lowest Zeeman triplet
condenses:
truncate Hilbert space

$$4^L \rightarrow 2^L$$



each ladder rung is either singlet or $S^Z = 1$: map to
fermions or hard core bosons or $S=1/2$

effective $S=1/2$ chain for two leg ladder is:

$$J_{\text{eff}}^{xy} = J_{\text{leg}}, \quad J_{\text{eff}}^z = \frac{1}{2} J_{\text{leg}}, \quad H_{\text{eff}} = H - \frac{1}{2} J_{\text{leg}} - J_{\text{rung}}$$

$J_{\text{eff}}^z < J_{\text{eff}}^{xy}$: intermediate phase is Luttinger liquid

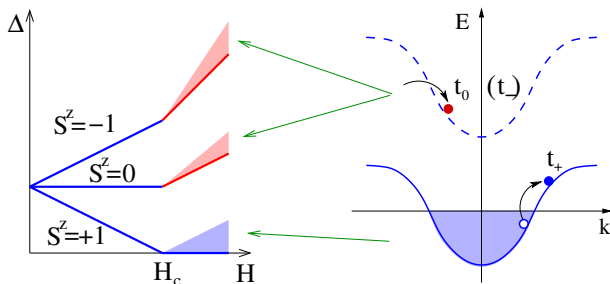
Mila '00 / Tsvelik and Giamarchi '03

► NDMAP

isotropic 1D system: critical phase

ground state band: map to fermions

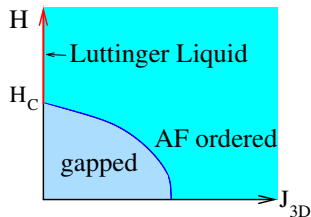
higher bands: “mobile impurities”

response: **edge singularities**, i.e. $S(q = \pi, \omega) \propto (\omega - \Delta_\mu)^{-\alpha}$ Fermi sea rearrangement \Rightarrow **change of slope at $H = H_c$**

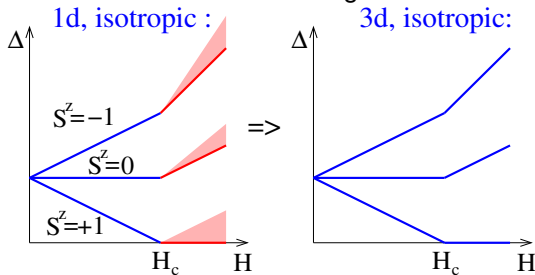
A.Furusaki & S.-C.Zhang '99 / A. Kolezhuk & HJM '02

3D interactions: critical phase becomes unstable

- U(1) *spontaneously* broken
field-induced AF order above H_c
- continua collapse
quasiparticle response



“Bose-Einstein condensation of magnons”



T.Nikuni et al. '00 / Ch.Rüegg et al. '03

► NDMAP

dimer field theory

Idea:

- take a generic **weakly coupled** system: $S = \frac{1}{2}$ dimer chain



- introduce anisotropy: $J_x S_1^x S_2^x + J_y S_1^y S_2^y + J_z S_1^z S_2^z$
- carry the results over to **strongly coupled** systems (e.g. $S = 1$ Haldane chain)

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Tool: dimer coherent states

(A. Kolezhuk '96)

$$|\Psi_{\text{dimer}}\rangle = \sqrt{1 - A^2 - B^2} |s\rangle + (\vec{A} + i\vec{B}) \cdot |\vec{t}\rangle$$

$$\langle \vec{S}_1 + \vec{S}_2 \rangle = 2(\vec{A} \times \vec{B}) \quad \mapsto \text{magnetization}$$

$$\langle \vec{S}_1 - \vec{S}_2 \rangle = 2\vec{A}\sqrt{1 - A^2 - B^2} \quad \mapsto \text{staggered magnetization}$$

$$\langle \vec{S}_1 \times \vec{S}_2 \rangle = \vec{B}\sqrt{1 - A^2 - B^2} \quad \mapsto \text{vector chirality}$$

dimer field theory Lagrangean:

- φ^4 -type theory for a **complex** bosonic field ($A, B \ll 1$) with
- **generally, two sets of “stiffness constants”**: $m_i \neq \tilde{m}_i$

$$\tilde{m}_x = \frac{1}{2}(J_y + J_z) \text{ etc.}, \quad m_i = \tilde{m}_i - J'$$

$$\lambda = J', \quad \lambda_1 = 2J', \quad \lambda_2 = -J'$$

► NDMAP

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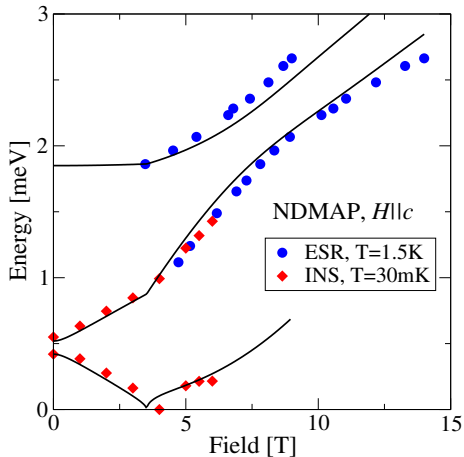
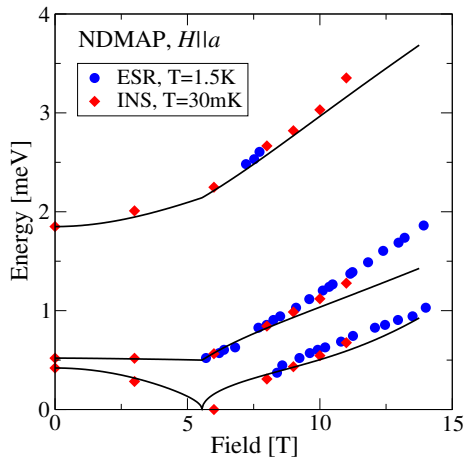
- effective Lagrangean after integrating out B :

$$\mathcal{L}_{\text{eff}} = \frac{1}{\tilde{m}_i} \{ \hbar^2 (\partial_t A_i)^2 - V_i^2 (\partial_x A_i)^2 \} - 2 \frac{\hbar}{\tilde{m}_i} (\vec{H} \times \vec{A})_i \partial_t A_i - U_2 - U_4$$

- **anisotropic Zeeman term** (due to \tilde{m}_i)
- **anisotropic interaction** at $H \neq 0$ (due to λ_1, λ_2)



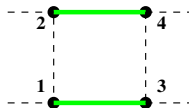
Application: $\text{Ni}(\text{C}_5\text{H}_{14}\text{N}_2)_2\text{N}_3(\text{PF}_6)$ (NDMAP)

Neutrons: [Zheludev et al.'03, '04](#)ESR: [Hagiwara et al. '03](#)[▶ \$\text{TiCuCl}_3\$](#) [◀ back](#)

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add four spin interactions

basic building block
of ladders and cuprates
is **plaquette with four spins**



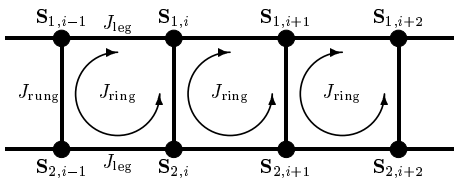
general plaquette hamiltonian has 9 parameters
(+ arbitrary constant):

6 **two spin** interactions: 2 rungs, 2 legs, 2 diagonals

3 **four spin** interactions: leg-leg, diagonal-diagonal, rung-rung

exact ground states exist for some parameter sets

a particular linear combination amounts to **cyclic (ring) exchange**:



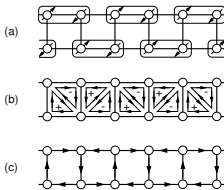
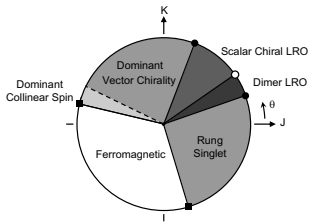
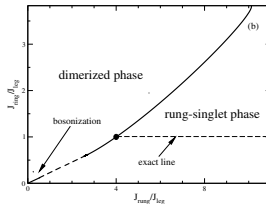
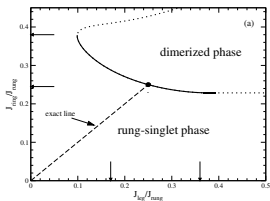
$$\mathcal{H} = \sum_{\text{plaquettes}} \frac{1}{2} J (P_{12} + P_{34}) + \frac{1}{2} J_{\text{leg}} (P_{13} + P_{24}) + \frac{1}{2} J_{\text{ring}} (P_{1243} + P_{1243}^{-1})$$

$$= \sum_{\text{plaquettes}} (J + J_{\text{ring}}) (\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_3 \cdot \vec{S}_4)$$

$$+ (J_{\text{leg}} + \frac{1}{2} J_{\text{ring}}) (\vec{S}_1 \cdot \vec{S}_3 + \vec{S}_2 \cdot \vec{S}_4) + \frac{1}{2} J_{\text{ring}} (\vec{S}_1 \cdot \vec{S}_4 + \vec{S}_2 \cdot \vec{S}_3)$$

$$+ 2J_{\text{ring}} \{ (\vec{S}_1 \cdot \vec{S}_2)(\vec{S}_3 \cdot \vec{S}_4) + (\vec{S}_1 \cdot \vec{S}_3)(\vec{S}_2 \cdot \vec{S}_4) - (\vec{S}_1 \cdot \vec{S}_4)(\vec{S}_2 \cdot \vec{S}_3) \}$$

phase diagram including ring exchange



staggered dimer

scalar chiral

vector chiral

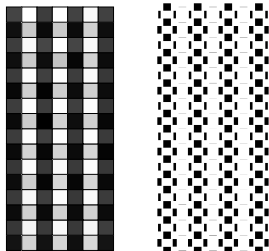
Müller, Vekua and HJM '02 / Läuchli, Schmid and Troyer '03

ring exchange in 2D

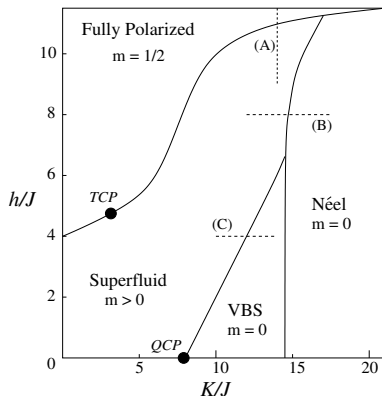
La_2CuO_4 : ring exchange required to describe the dispersion of zone boundary magnons

$S=1/2$ model with ring exchange:

ring exchange introduces new quantum phases



Sandvik et al. '02 / '04



xy=superfluid phase • striped = VBS phase • Neel phase

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from Ising domain walls to isotropic spinons

start from Ising limit

$$\mathcal{H} = \frac{1}{2} J \sum \sigma_n^z \sigma_{n+1}^z$$

ground state $\uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \dots$

excited states:

domain wall $\uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \dots$

$$\Delta E = |J|$$

spin clusters $\uparrow \downarrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow \uparrow \downarrow \dots$

$$\Delta E = 2|J|$$

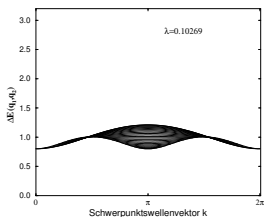
$\uparrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \dots$

domain wall = soliton
 \rightarrow spinon

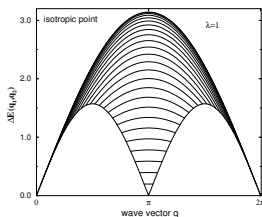
- spin cluster = 'spin wave'
 = two spinon continuum

spinon continua in $S=1/2$ chains

\approx Ising limit

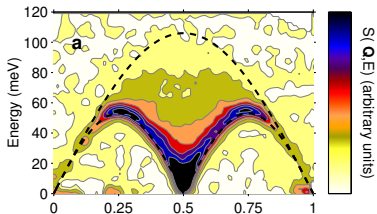


Heisenberg limit



KCuF_3 , $S=1/2$:

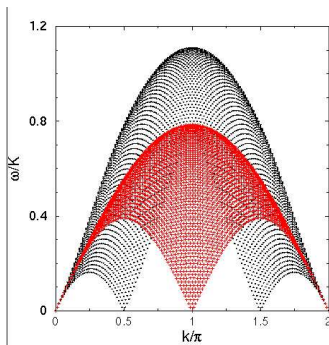
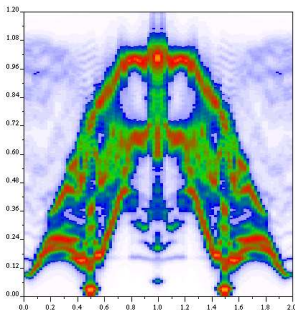
B. Lake, A. Tennant, Nature Materials 2004



3 sets of spinons at the SU(4) point

SU(4) symmetric Kugel-Khomskii model: $J_S = J_T = K/4$ in

$$\mathcal{H} = J_S \sum_n (\mathbf{S}_n \cdot \mathbf{S}_{n+1}) + J_T \sum_n (\mathbf{T}_n \cdot \mathbf{T}_{n+1}) \\ + K \sum_n (\mathbf{S}_n \cdot \mathbf{S}_{n+1})(\mathbf{T}_n \cdot \mathbf{T}_{n+1})$$



Affleck '89, Schollwöck '00

- 1 Introduction
- 2 prototypes of low D magnets
- 3 low D quantum magnets in an external magnetic field
- 4 multi spin interactions
- 5 excitation continua
- 6 Summary**

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Low D quantum magnets with general exchange interactions cover a vast number of materials and theoretical models.

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Challenges:

- Experiment: new materials / high magnetic fields
- Theory: 2D / symmetries and quantum phases

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H. Tanaka, A. Oosawa, TIT

M. Matsuda, K. Katsumata, H. Hagiwara, Z. Honda, RIKEN

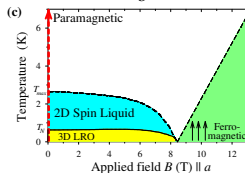
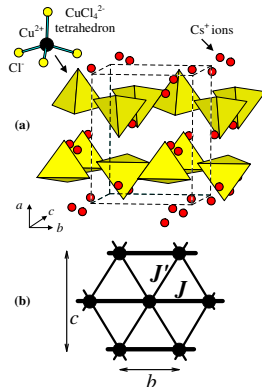
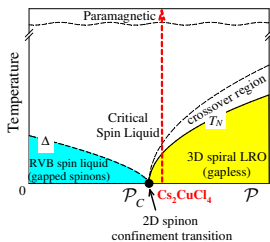
A. Zheludev, Oak Ridge

HJM and AK Kolezhuk, One-dimensional Magnetism

review article in: Quantum Magnetism, Lect. Notes Phys. **645**, 1 (2004)

Cs₂CuCl₄ phase diagrams

← back



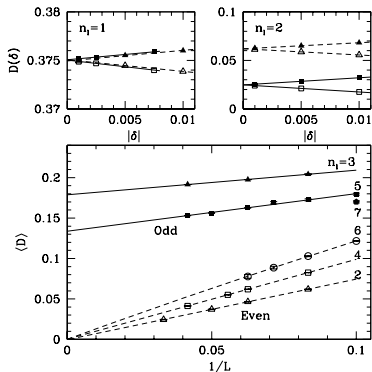
purists' view of a spin liquid

spin liquid requires:

no spontaneous dimerization
(Majumdar-Ghosh disqualifies)

only one electron per unit cell
(ladder and $S=1$ chain disqualify)

purists' example is (Capriotti):
even leg ladder / 2D HAF
with NN and NNN exchange:
gs not dimerized



dimer susceptibility

◀ back

L. Capriotti, D.J. Scalapino and S.R. White, PRL '04

dimer field theory Lagrangean:

- a φ^4 -type theory for a **complex** bosonic field ($A, B \ll 1$)

$$\begin{aligned} \mathcal{L} = & \hbar \left(\vec{A} \cdot \frac{\partial \vec{B}}{\partial t} - \vec{B} \cdot \frac{\partial \vec{A}}{\partial t} \right) - \frac{1}{2} J' \left(\frac{\partial \vec{A}}{\partial x} \right)^2 - m_i A_i^2 - \tilde{m}_i B_i^2 \\ & + 2\vec{H} \cdot (\vec{A} \times \vec{B}) - \lambda A^4 - \lambda_1 (A^2 B^2) - \lambda_2 (\vec{A} \cdot \vec{B})^2 \end{aligned}$$

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- **generally, two sets of “stiffness constants”**: $m_i \neq \tilde{m}_i$

$$\tilde{m}_x = \frac{1}{2}(J_y + J_z) \text{ etc.}, \quad m_i = \tilde{m}_i - J'$$

$$\lambda = J', \quad \lambda_1 = 2J', \quad \lambda_2 = -J'$$

effective Lagrangean for real field \vec{A} :

◀ back

$$\vec{B} = \hat{Q}\vec{F}, \quad \vec{F} = -\hbar \frac{\partial \vec{A}}{\partial t} + (\vec{H} \times \vec{A}), \quad Q_{ij} = \frac{\delta_{ij}}{\tilde{m}_i} - \lambda_1 \frac{\delta_{ij} \vec{A}^2}{\tilde{m}_i^2} - \lambda_2 \frac{A_i A_j}{\tilde{m}_i \tilde{m}_j}$$

$$\mathcal{L}_{\text{eff}} = \frac{1}{\tilde{m}_i} \left\{ \hbar^2 \left(\frac{\partial A_i}{\partial t} \right)^2 - V_i^2 \left(\frac{\partial A_i}{\partial x} \right)^2 \right\} - 2 \frac{\hbar}{\tilde{m}_i} (\vec{H} \times \vec{A})_i \frac{\partial A_i}{\partial t} - U_2 - U_4$$

here $U_2(\vec{A}) = m_i A_i^2 - \frac{1}{\tilde{m}_i} (\vec{H} \times \vec{A})_i^2$

$$U_4(\vec{A}, \frac{\partial \vec{A}}{\partial t}) = \lambda A^4 + \lambda_1 A^2 \frac{1}{\tilde{m}_i^2} F_i^2 + \lambda_2 \frac{A_i A_j}{\tilde{m}_i \tilde{m}_j} F_i F_j$$

Some properties of the model:

- zero-field gaps: $\Delta_z = \sqrt{m_z \tilde{m}_z}$ etc.
- critical fields: $H_c^{(z)} = \min \left\{ \sqrt{m_x \tilde{m}_y}, \sqrt{\tilde{m}_x m_y} \right\}$ etc.
- reduces to known theories in limiting special cases:

$$\tilde{m}_i = \tilde{m} \quad \Rightarrow \quad \text{Affleck} \quad H_c^{(z)} = \Delta_z$$

$$\tilde{m}_i = m_i = \Delta_i \quad \Rightarrow \quad \text{Mitra\&Halperin} \quad H_c^{(z)} = \sqrt{\Delta_x \Delta_y}$$

- **allows to avoid the OP direction problem**



How many fitting parameters?

nine constants present in the theory:

$$\lambda, \quad \lambda_{1,2}, \quad m_{x,y,z}, \quad \tilde{m}_{x,y,z}$$

but only **three** are left if we fix critical fields and zero-field gaps:

- six equations

$$\begin{aligned} H_{c,z}^2 &= m_x \tilde{m}_y, & H_{c,x}^2 &= m_y \tilde{m}_z, & H_{c,y}^2 &= m_x \tilde{m}_z, \\ \Delta_z^2 &= m_z \tilde{m}_z, & \Delta_x^2 &= m_x \tilde{m}_x, & \Delta_y^2 &= m_y \tilde{m}_y \end{aligned}$$

define five independent constraints, so from $(m_{x,y,z}, \tilde{m}_{x,y,z})$ only one parameter is free (overall scale)

- mode energies depend only on the **ratios** $\lambda_1/\lambda, \quad \lambda_2/\lambda$

The OP direction at $H > H_c$

◀ back

- in Mitra&Halperin, for $\vec{H} \parallel z$: **inherent problem**

$$U_2 = \left(\Delta_x - \frac{H^2}{\Delta_y}\right) A_x^2 + \left(\Delta_y - \frac{H^2}{\Delta_x}\right) A_y^2 + \Delta_z A_z^2,$$

if $\Delta_x < \Delta_y$ ($x = \text{easy axis}$) then $\vec{A} \parallel \vec{y}$ for $H > H_c$

i.e. the staggered order *always along the harder axis!*

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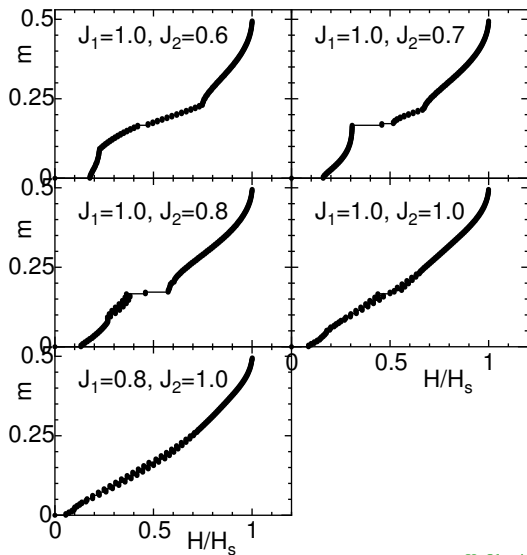
- not the case for the proposed theory:**

$$U_2 = \left(m_x - \frac{H^2}{\tilde{m}_y}\right) A_x^2 + \left(m_y - \frac{H^2}{\tilde{m}_x}\right) A_y^2 + m_z A_z^2,$$

if $m_x/\tilde{m}_x < m_y/\tilde{m}_y$ then $\vec{A} \parallel \vec{x}$, $H_c = \sqrt{m_x \tilde{m}_y}$

if $m_x/\tilde{m}_x > m_y/\tilde{m}_y$ then $\vec{A} \parallel \vec{y}$, $H_c = \sqrt{m_y \tilde{m}_x}$

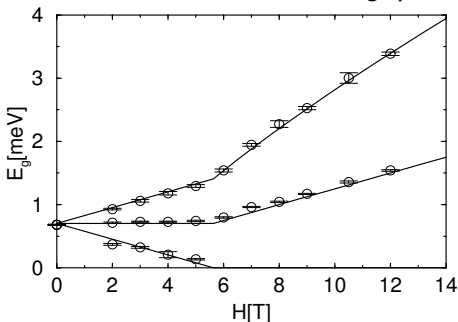
magnetization plateau in the NN-NNN chain



K. Okunishi and T. Tonegawa, JPSJ 72, 479 (2003)

Application: TlCuCl_3 (3D-coupled $S = \frac{1}{2}$ dimers)

- INS (Rüegg et al '03): the lowest mode is gapless (“BEC”)?



- ESR Glazkov et al. '03: gap reopens at $H > H_c \Rightarrow$ **anisotropy!**
- consistent with exchange anisotropy $< 1\%$ (intra- and inter-dimer)

